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Dmitri V. Alexandrov, Alexander A. Ivanov, and Irina V. Alexandrova

Analytical Solution to the Equations of a Two-Phase Layer with Allowance for the Convective Heat and Mass Transfer in a Binary Liquid

Dmitri V. Alexandrov[a)], Alexander A. Ivanov[b)] and Irina V. Alexandrova[c)]

Department of Theoretical and Mathematical Physics, Laboratory of Multi-Scale Mathematical Modeling, Ural Federal University, Ekaterinburg 620000, Russian Federation

[a)]Corresponding author: dmitri.alexandrovr@urfu.ru
[b)]alexandr.a.ivanov@bk.ru
[c)]irina.alexanderova@urfu.ru

Abstract. The model equations describing directional crystallization of a binary system with a two-phase layer and taking into account the convective heat and mass transfer mechanism in the liquid phase are formulated. The system of formulated nonlinear heat and mass transfer equations is solved analytically in the case of steady-state crystallization scenario. The temperature and concentration distributions, the solid phase fraction, the two-phase layer thickness and its boundaries, solid phase - mushy layer and mushy layer - liquid phase, are found. The steady-state crystallization velocity is determined as a function of fixed model parameters. The developed model and its analytical solutions describe the case of intensive motions of a binary liquid (the case of turbulent flows in the ocean, for example).

INTRODUCTION

The processes of directional and bulk crystallization are often encountered in the description of liquid-solid phase transformations in materials science and geophysics [1–7]. A large number of such processes occur in the presence of a supercooled two-phase region, where the process of phase transformation from a liquid to a solid state occurs [8–12]. This region is filled with a liquid phase (supercooled melt, supersaturated solution) and a solid phase growing in the form of dendrite-like structures. The mathematical description of such a two-phase region consists of a system of nonlinear differential equations, as well as boundary conditions imposed on the moving boundaries of phase transformation: solid phase - two-phase region and two-phase region - liquid phase. In papers [13–17], the analytical solutions were constructed for the nonlinear system of equations of the two-phase region under conditions of a quasistationary crystallization in the case of conductive boundary conditions of heat and mass balance. The self-similar solutions (when the crystallization rate is inversely proportional to the square root of time) in the case of conductive boundary conditions were found in papers [18–21]. Then, in papers, [22–25], approximate analytical and numerical solutions of the nonlinear system of equations of the two-phase zone were determined under unsteady crystallization conditions. However, with intensive mixing of the liquid phase, the heat and mass fluxes at the boundary between the two-phase region and liquid are determined by the intensity of convection. In this case, it is necessary to use the boundary conditions of the convective type (taking into account convective heat and mass fluxes) [26–28]. The present paper is devoted to exact analytical solutions of nonlinear heat and mass transfer equations that describe the steady-state solidification scenario with convective boundary conditions at the two-phase region - liquid phase boundary.

THE MODEL

We consider the steady-state process of binary melt crystallization along the spatial coordinate ξ (Fig. 1). The phase transformation region is divided into three domains occupied by the solid phase ($\xi < u_s\tau$), the two-phase region ($u_s\tau < \xi < u_s\tau + \delta$), and the liquid phase ($\xi > u_s\tau + \delta$), where u_s and δ are the constant crystallization velocity and

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thickness of the two-phase layer. We consider the quasi-equilibrium model of the two-phase region, i.e. the model where the growing solid phase releases the latent heat of solidification and completely compensates the constitutional supercooling. In this case, the system of heat and mass transfer equations in the two-phase layer takes the form [29]

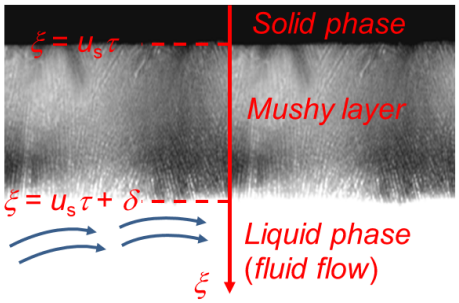

Figure 1. A scheme of crystallization process with a two-phase layer.

$$\frac{\partial}{\partial\tau}\left[(1-\varphi)\,\sigma\right] = \frac{\partial}{\partial\xi}\left(D(\varphi)\frac{\partial\sigma}{\partial\xi}\right) - k\sigma\frac{\partial\varphi}{\partial\tau}, \quad u_s\tau < \xi < u_s\tau + \delta, \tag{1}$$

$$\frac{\partial}{\partial\xi}\left(\lambda(\varphi)\frac{\partial\theta}{\partial\xi}\right) + \rho L\frac{\partial\varphi}{\partial\tau} = 0, \quad u_s\tau < \xi < u_s\tau + \delta, \tag{2}$$

$$\theta = \theta_0 - m\sigma, \quad u_s\tau < \xi < u_s\tau + \delta, \tag{3}$$

where θ and σ represent the temperature and impurity concentration in the two-phase region, φ is the solid fraction, τ is the time, k is the equilibrium partition coefficient, ρ is the density of solid phase, L is the latent heat of crystallization, θ_0 is the phase transition temperature of pure melt (when $\sigma = 0$), m is the liquidus slope, and coefficients $D(\varphi)$ and $\lambda(\varphi)$ represent the linear functions of the solid phase fraction, i.e.

$$D(\varphi) = D_l(1-\varphi), \quad \lambda(\varphi) = \lambda_l(1-\varphi) + \lambda_s\varphi. \tag{4}$$

Here D_l is the diffusion coefficient, and λ_l and λ_s are the thermal conductivities in the liquid and solid phases, respectively.

We consider the case when the temperature gradient in the solid phase g_s is fixed, i.e.

$$\frac{\partial\theta_s}{\partial\xi} = g_s, \quad \xi < u_s\tau. \tag{5}$$

Here θ_s stands for the temperature in the solid phase.

At the boundary $\xi = u_s\tau$ between the solid phase and two-phase domain, we have classical heat and mass balance conditions

$$\lambda_s g_s - \lambda(\varphi_*)\frac{\partial\theta}{\partial\xi} = \rho L(1-\varphi_*)u_s, \quad \varphi = \varphi_*, \quad \xi = u_s\tau, \tag{6}$$

$$(1-k)(1-\varphi_*)\sigma u_s + D(\varphi_*)\frac{\partial\sigma}{\partial\xi} = 0, \quad \xi = u_s\tau, \tag{7}$$

where φ_* is the solid fraction at $\xi = u_s\tau$.

At the boundary $\xi = u_s\tau + \delta$ between the two-phase region and liquid phase, let us write down the following convective heat and mass transfer boundary conditions [26–28]

$$\varphi = 0, \quad \sigma = \sigma_b, \quad \theta = \theta_b, \quad \xi = u_s\tau + \delta, \tag{8}$$

$$\lambda_l\frac{\partial\theta}{\partial\xi} = \alpha_h\rho_l c_l u(\theta_\infty - \theta_b), \quad D_l\frac{\partial\sigma}{\partial\xi} = \alpha_s u(\sigma_\infty - \sigma_b), \quad \xi = u_s\tau + \delta, \tag{9}$$

where θ_b and σ_b designate the boundary values of temperature and impurity concentration (at $\xi = u_s\tau + \delta$), θ_∞ and σ_∞ are the temperature and concentration in liquid far from the boundary $\xi = u_s\tau + \delta$, α_h and α_s are the convective transfer coefficients for heat and mass, ρ_l and c_l are the density and specific heat of the liquid phase, and u is the fricti6ion velocity. The ratio of transfer coefficients is experimentally known in the form $\alpha_h/\alpha_s = (a_l/D_l)^n$, where $2/3 < n < 4/5$ [30–32] (a_l stands for the thermal diffusivity in liquid).

In addition, the temperature and concentration fields in liquid far from the boundary $\xi = u_s\tau + \delta$ are regarded as known

$$\theta_l \to \theta_\infty, \;\; \sigma_l \to \sigma_\infty, \;\; \xi \to \infty. \tag{10}$$

Below we construct the exact analytical solution of nonlinear system (1)-(10) in a parametric form.

ANALYTICAL SOLUTIONS

Let us now introduce the following dimensionless variables and parameters

$$x = \frac{u_s}{D_l}(\xi - u_s\tau), \;\; \varepsilon = \frac{u_s\delta}{D_l}, \;\; T = \frac{\theta}{m\sigma_\infty}, \;\; C = \frac{\sigma}{\sigma_\infty}, \;\; P = \frac{\lambda_s m\sigma_\infty}{\rho L D_l}, \;\; T_b = \frac{\theta_b}{m\sigma_\infty}, \;\; C_b = \frac{\sigma_b}{\sigma_\infty}, \tag{11}$$

$$T_\infty = \frac{\theta_\infty}{m\sigma_\infty}, \;\; T_0 = \frac{\theta_0}{m\sigma_\infty}, \;\; \Lambda_0(\varphi) = \frac{\lambda(\varphi)}{\lambda_s}, \;\; R_h = \frac{\alpha_h\rho_l c_l u D_l}{u_s\lambda_l}, \;\; R_s = \frac{\alpha_s u}{u_s}. \tag{12}$$

Equations (1)-(3) in dimensionless variables (11) and (12) become

$$\frac{d}{d\varphi}\left[(1-\varphi)C - \Xi(\varphi)\right] + kC = 0, \;\; 0 < x < \varepsilon, \tag{13}$$

$$\Lambda_0(\varphi)\frac{dT}{dx} = \frac{\varphi}{P} + A, \;\; 0 < x < \varepsilon, \tag{14}$$

$$T = T_0 - C, \;\; 0 < x < \varepsilon, \tag{15}$$

where A is a constant of integration, and

$$\Xi(\varphi) = \frac{1-\varphi}{\Lambda_0(\varphi)}\left(\frac{\varphi}{P} + A\right).$$

Note that when deriving equation (13) it was taken into account that

$$\frac{dC}{dx} = -\frac{dT}{dx} = -\frac{1}{\Lambda_0(\varphi)}\left(\frac{\varphi}{P} + A\right), \;\; 0 < x < \varepsilon \tag{16}$$

following from equations (14) and (15). An important point is that the impurity concentration C in the two-phase region $0 < x < \varepsilon$ is only a function of the solid fraction φ (this conclusion follows from equation (13)).

Integrating equation (13) and taking into account that $C = C_b$ at $\varphi = 0$ (at $x = \varepsilon$), we have the impurity concentration in the two-phase region

$$C(\varphi) = \left[C_b + \int_0^\varphi \frac{\Xi'(\tilde{\varphi})d\tilde{\varphi}}{(1-\tilde{\varphi})^k}\right](1-\varphi)^{k-1}, \;\; 0 < x < \varepsilon, \tag{17}$$

where $\Xi'(\tilde{\varphi}) = d\Xi/d\tilde{\varphi}$.

The boundary conditions (8) and (9) in dimensionless variables (11) and (12) lead to the following conditions

$$\frac{dT}{dx} = R_h(T_\infty - T_b), \;\; \frac{dC}{dx} = R_s(1 - C_b), \;\; x = \varepsilon, \;\; \varphi = 0. \tag{18}$$

Now combining (15), (16) and (18), we determine the boundary values of temperature and impurity concentration (at $x = \varepsilon$ or $\varphi = 0$)

$$T_b = \frac{R_h T_\infty + R_s(1 - T_0)}{R_h - R_s}, \;\; C_b = T_0 - T_b. \tag{19}$$

Substitution of expression (14) into the first condition (18) at $\varphi = 0$ gives constant A

$$A = \Lambda_1 R_h (T_\infty - T_b), \quad \Lambda_1 = \frac{\lambda_l}{\lambda_s}.$$

Now the boundary condition (6) enables us to find the steady-state crystallization velocity u_s in the form

$$u_s = \frac{\lambda_s (g_s - g_l)}{\rho L}, \quad g_l = \frac{u_s m \sigma_\infty \Lambda_1 R_h (T_\infty - T_b)}{D_l}. \tag{20}$$

Combining expressions (7), (14) and (16), we come to the equation for the solid fraction φ_* at the boundary solid phase - two-phase region

$$(1-k)C(\varphi_*) - \frac{\varphi_* + AP}{P\Lambda_0(\varphi_*)} = 0. \tag{21}$$

Keeping in mind that

$$\frac{dC}{dx} = \frac{dC}{d\varphi}\frac{d\varphi}{dx} = -\frac{\varphi + AP}{P\Lambda_0(\varphi)}$$

(see expression (16)), we arrive at the function

$$x(\varphi) = \varepsilon - \int_0^\varphi \frac{P\Lambda_0(\tilde{\varphi})C'(\tilde{\varphi})}{\tilde{\varphi} + AP} d\tilde{\varphi}, \quad 0 < x < \varepsilon. \tag{22}$$

The dimensionless two-phase region thickness ε is determined from expression (22) by means of substitution $x = 0$ at $\varphi = \varphi_*$ ant takes the form

$$\varepsilon = \int_0^{\varphi_*} \frac{P\Lambda_0(\tilde{\varphi})C'(\tilde{\varphi})}{\tilde{\varphi} + AP} d\tilde{\varphi}. \tag{23}$$

Note that $C'(\tilde{\varphi}) = dC/d\tilde{\varphi}$ is given by expression (17).

Now expressions (17)-(23) determine the exact analytical solution of the nonlinear problem on crystallization with a two-phase region in a parametric form (with parameter φ). Let us also emphasize that the crystallization velocity can be found from expression (20) in an explicit form after substituting $R_h(u_s)$ from (12) as

$$u_s = \frac{\lambda_s g_s - (T_\infty - T_b)\alpha_h \rho_l c_l u m \sigma_\infty}{\rho L}. \tag{24}$$

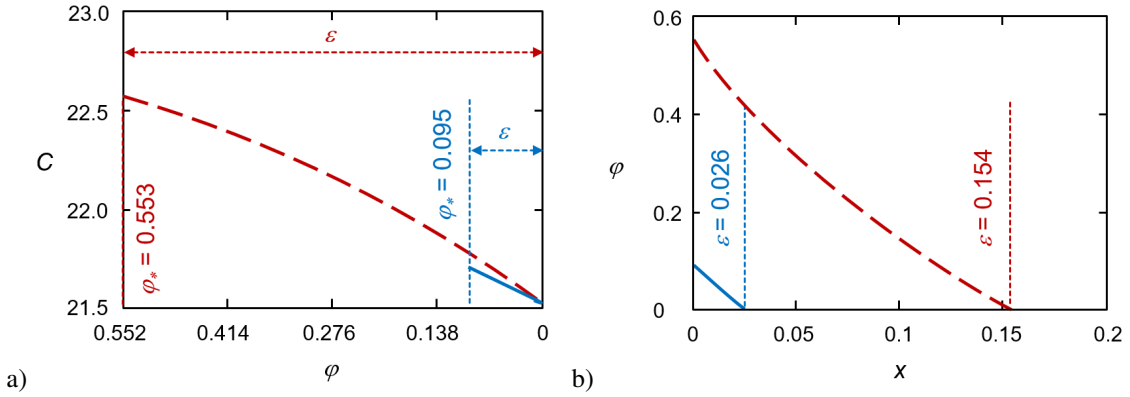

Figure 2. The concentration of impurity as a function of the solid phase fraction (a) and the solid phase fraction as a function of spatial coordinate (b) at different friction velocities: $u = 0.3$ m/s (dashed lines) and $u = 0.29$ m/s (solid lines).

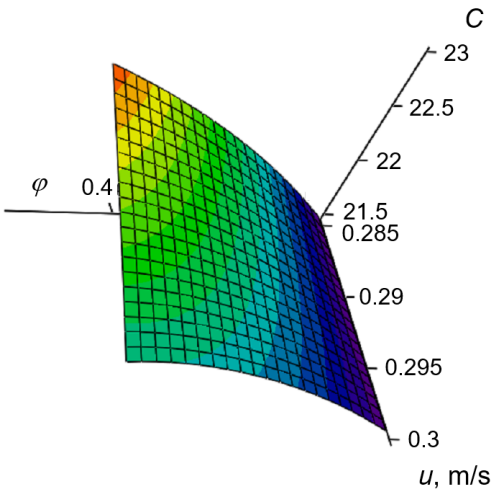

Figure 3. The concentration of impurity in the two-phase region as a function of the solid phase fraction and friction velocity.

CONCLUSIONS

Figures 2 and 3 show the analytical solution plotted in accordance with expressions (17)-(24). Here it is easily seen that the impurity concentration C and the solid phase fraction φ are the decreasing functions within a two-phase layer. So, for instance, the fraction φ reduces from a certain value φ_* at the solid phase - two-phase layer boundary ($x = 0$) to zero at the two-phase layer - liquid phase boundary ($x = \varepsilon$). In addition, the thickness of the two-phase layer increases with increasing the friction velocity u. As this takes place, the boundary values of C and φ at $x = 0$ increase too.

Let us especially note in conclusion that the present theory of quasiequilibrium crystallization should be extended having regard to the processes of nucleation and crystal growth in a two-phase layer recently described in papers [33–37].

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